Simulation of an entangled state in a chain of three nuclear spins system

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ABSTRACT

We study the formation of an entangled state in a one-dimensional chain of three nuclear spins system which interact weakly through the Ising type of interaction and taking into account first and second neighbor interactions. We can get this entangled state using two pulses ($\pi/2$ and π pulses), and we study the efficiency of getting this entangled state as a function of the ratio of the second neighbor interaction coupling constant to the first neighbor interaction coupling constant (J'/J). We found that for $J'/J \geq 0.04$, the entangled state is well defined.

1. Introduction

The huge interest in quantum computation and quantum information was triggered by the polynomial time solution of the prime factorization problem (Shor's algorithm [1]), the fast data base searching (Grover's algorithm [2]), error correction codes [3], robust entanglement [4], and the teleportation phenomenum [5]. Almost any quantum system with at least two quantum levels may be used, in principle, for quantum computation. This one uses qubits (quantum bits) instead of bits to process information. A qubit is the superposition of any two levels of the system , called $|0\rangle$ and $|1\rangle$ states, $\Psi = C_0|0\rangle + C_1|1\rangle$ with $|C_0|^2 + |C_1|^2 = 1$. The tensorial product of L-qubits makes up a register of lenght L, say $|x\rangle = |i_{L-1}, \ldots, i_0\rangle$, with $i_j = 0, 1$, and a quantum computer with L-qubits works in a 2^L dimensional Hilbert space, where an element of this space is of the form $\Psi = \sum C_x|x\rangle$, with $\sum |C_x|^2 = 1$.

Quantum computers of few qubits [6] have been in operations and have been used to explore quantum gates, entanglement, small number Shor's factorization, small data base Grover's searching, teleportation, error corrections, and cryptography. However, to make serious computer calculations one may requires a quantum computer with at least of 100-qubits registers, and we think that will be hopefully achived in a near future. One solid state quantum comuter model that has been explored for physical realization and which allows to make analytical studies is that one made up by one-dimensional chain of nuclear spins sytems [7] , where the Ising interaction among first neighbor spins allows to inplement ideally this type of computer with 1000-qubits or more [8]. One of the important phenomena we studied with this model was the entangled state formation [9]. In this paper, we consider second neighbor spin interaction in a chain of three nuclear spins system. We show that this allows us to implement an entangled state using two pulses ($\pi/2$ and π), and we determine the threshold of the second neighbor interaction coupling parameter to get a well define entangled state.

2. Equation of Motion

Consider a one-dimensional chain of three equally spaced nuclear-spins system (spin one half) making an angle $\cos\theta = 1/\sqrt{3}$ with respect the z-component of the magnetic field (selected in this way to eliminate the dipole-dipole interaction between spins) and having an rf-magnetic field in the transversal plane. The magnetic field is given by

$$\mathbf{B} = (b\cos(\omega t + \varphi), -b\sin(\omega t + \varphi), B_o(z)) \ , \tag{1}$$

where b is the amplitude of the rf-field, $B_o(z)$ is the amplitude of the z-component of the magnetic field, ω and φ are the angular frequency and phase of the rf-field. So, the Hamiltonian of the system is given by

$$H = -\sum_{k=0}^{2} \mu_{\mathbf{k}} \cdot \mathbf{B}_{\mathbf{k}} - 2J\hbar \sum_{k=0}^{1} I_k^z I_{k+1}^z - 2J'\hbar \sum_{k=0}^{0} I_k^z I_{k+2}^z \ , \tag{2}$$

where $\mu_{\mathbf{k}}$ represents the magnetic moment of the kth-nucleus which is given in terms of the nuclear spin as $\mu_{\mathbf{k}} = \hbar\gamma(I_k^x, I_k^y, I_k^z)$, being γ the proton gyromagnetic ratio. $\mathbf{B_k}$ represents the magnetic field at the location of the kth-spin ($z = z_k$). The

second term at the right side of (2) represents the first neighbor spin interaction, and the third term represents the second neighbor spin interaction. J and J' are the coupling constants for these interactions. This Hamiltonian can be written in the following way

$$H = H_0 + W \ , \tag{3a}$$

where H_0 and W are given by

$$H_0 = -\hbar \left\{ \sum_{k=0}^{2} \omega_k I_k^z + 2J(I_0^z I_1^z + I_1^z I_2^z) + 2J' I_0^z I_2^z \right\} \tag{3b}$$

and

$$W = -\frac{\hbar\Omega}{2} \sum_{k=0}^{2} \left[e^{i(\omega t+\varphi)} I_k^+ + e^{-i(\omega t+\varphi)} I_k^- \right] \ , \tag{3c}$$

where $\omega_k = \gamma B_o(z_k)$ is the Larmore frequency of the kth-spin, $\Omega = \gamma b$ is the Rabi's frequency, and $I_k^{\pm} = I_k^x \pm i I_k^y$ represents the ascend operator (+) or the descend operator (-). The Hamiltonian H_0 is diagonal on the basis $\{|i_2 i_1 i_0\rangle\}$, where $i_j = 0, 1$ (0 for the ground state and 1 for the exited state),

$$H_0 |i_2 i_1 i_0\rangle = E_{i_2 i_1 i_0} |i_2 i_1 i_0\rangle \ . \tag{4a}$$

The eigenvalues $E_{i_2 i_1 i_0}$ are given by

$$E_{i_2 i_1 i_0} = -\frac{\hbar}{2} \Big\{ (-1)^{i_2}\omega_2 + (-)^{i_1}\omega_1 + (-1)^{i_0}\omega_0 + J[(-1)^{i_0+i_1} + (-1)^{i_1+i_2}] + (-1)^{i_0+i_2} J' \Big\} . \tag{4b}$$

The term (3c) of the Hamiltonian (3a) allows to have a single spin transitions on the above eigenstates by choosing the proper resonant frequency, as shown in Figure 1. In this work, we are interested in the transitions $|000\rangle \longleftrightarrow |001\rangle$ and $|001\rangle \longleftrightarrow |101\rangle$ which have the resonant frequencies

$$\omega = \omega_0 + J + J' \tag{5a}$$

and

$$\omega = \omega_2 + J - J' \ . \tag{5b}$$

To solve the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi \ , \tag{6}$$

let us propose a solution of the form

$$\Psi(t) = \sum_{k=0}^{7} C_k(t) |k\rangle \ , \tag{6}$$

where we have used decimal notation for the eigenstates in (4a), $H_0|k\rangle = E_k|k\rangle$. Substituting (6) in (5), multiplying for the bra $\langle m|$, and using the orthogonality relation $\langle m|k\rangle = \delta_{mk}$, we get the following equation for the coefficients

$$i\hbar \dot{C}_m = E_m C_m + \sum_{k=0}^{7} C_k \langle m|W|k\rangle \quad m = 0, \ldots, 7. \tag{7}$$

Now, using the following transformation

$$C_m(t) = D_m(t)e^{-iE_m t/\hbar} \ , \tag{8}$$

the fast oscillation term $E_m C_m$ of Eq. (7) is removed (this is equivalent to going to the interaction representation), and the following equation is gotten for the coefficients D_m

$$i\dot{D}_m = \frac{1}{\hbar}\sum_{k=0}^{7} W_{mk} D_k e^{i\omega_{mk}t} \ , \tag{9a}$$

where W_{mk} denotes the matrix elements $\langle m|W|k\rangle$, and ω_{mk} are defined as

$$\omega_{mk} = \frac{E_m - E_k}{\hbar} \ . \tag{9b}$$

Eq. (9a) represents a set of sixteen real coupling ordinary differential equations which can be solved numerically, and where W_{mk} are the elements of the matrix

$$(W) = -\frac{\hbar\Omega}{2}\begin{pmatrix} 0 & z^* & z^* & 0 & z^* & 0 & 0 & 0 \\ z & 0 & 0 & z^* & 0 & z^* & 0 & 0 \\ z & 0 & 0 & z^* & 0 & 0 & z^* & 0 \\ 0 & z & z & 0 & 0 & 0 & 0 & z^* \\ z & 0 & 0 & 0 & 0 & z^* & z^* & 0 \\ 0 & z & 0 & 0 & z & 0 & 0 & z^* \\ 0 & 0 & z & 0 & z & 0 & 0 & z^* \\ 0 & 0 & 0 & z & 0 & z & z & 0 \end{pmatrix} \ , \tag{9c}$$

where z is defined as $z = e^{i(\omega t+\varphi)}$, and z^* is its complex conjugated.

3. Numerical Simulations

We start with the ground state, $\Psi_0 = |000\rangle$, of the system and apply a $\pi/2$-pulse with $\varphi = 0$ and with frequency $\omega = \omega_0 - J - J'$ to get the superposition state

$$\Psi_1 = \frac{1}{\sqrt{2}}\Big(|000\rangle + |001\rangle\Big) \ . \tag{10}$$

Then, we apply a π-pulse with $\varphi = 0$ and frequency $\omega = \omega_2 + J - J'$ to get the entangled state

$$\Psi_2 = \frac{1}{\sqrt{2}}\Big(|000\rangle - |101\rangle\Big) \ . \tag{11}$$

The entangled state with plus sign can be gotten using a phase $\varphi = \pi$. To solve numerically (9a), we select similar values for the parameters as reference 8 and 9. So, in units of $2\pi \times MHz$, we set the following values

$$\omega_0 = 100 \ , \ \omega_1 = 200 \ , \ \omega_2 = 400 \ , \ J = 5 \ , \ \Omega = 0.1 \tag{12}$$

The coupling constant J' is chosen with at least one order of magnitude less that J since in the chain of spins one expect that second neighbor contribution to be at least one order of magnitude weaker than first neighbor contribution, depending on

the interspace separation of the nuclei. In all our simulations the total probability, $\sum |C_k(t)|^2$, is conserved equal to one within a precision of 10^{-6}.

Figure 2 shows the behavior of $Re\ D_0$, $Im\ D_0$, $Re\ D_5$, and $Im\ D_5$ during the two pulses ($t = \tau = \pi/2\Omega + \pi/\Omega$) for the digital initial state and with $J' = 0.2$. We can see the formation of the superposition state after the first $\pi/2$-pulse and the formation of the entangled state (11) after the following π-pulse. Fig. 3 shows the behavior of the probabilities $|C_k|^2$, $k = 0, \ldots, 7$ during the two pulses with the clear formation of the superposition state and the entangled state. Fig. 4 shows the behavior of the expected z-component of the spin,

$$\langle I_0^z \rangle = \frac{1}{2} \sum_{k=0}^{7} (-1)^k |C_k(t)|^2 \ , \tag{13a}$$

$$\langle I_1^z \rangle = \frac{1}{2} \Big\{ |C_0|^2 + |C_1|^2 - |C_2|^2 - |C_3|^2 + |C_4|^2 + |C_5|^2 - |C_6|^2 - |C_7|^2 \Big\} \ , \tag{13b}$$

and

$$\langle I_2^z \rangle = \frac{1}{2} \sum_{k=0}^{3} |C_k|^2 - \sum_{k=4}^{7} |C_k|^2 \ , \tag{13c}$$

during the two pulses. As one could expect $\langle I_0^z \rangle = \langle I_2^z \rangle = 0$ at the end of the two pulses due to the formation of the entangled state (11). The expected value of the spin is rotating in the plane (x, y) as is shown on Fig. 5. These transversal expected values are given by

$$\langle I_0^x \rangle = Re\Big(C_1^* C_0 + C_3^* C_2 + C_5^* C_4 + C_7^* C_6 \Big) \ , \qquad \langle I_0^y \rangle = Im\Big(\ldots \Big) \ , \tag{14a}$$

$$\langle I_1^x \rangle = Re\Big(C_2^* C_0 + C_3^* C_1 + C_6^* C_4 + C_7^* C_5 \Big) \ , \qquad \langle I_1^y \rangle = Im\Big(\ldots \Big) \ , \tag{14b}$$

and

$$\langle I_2^x \rangle = Re\Big(C_4^* C_0 + C_5^* C_1 + C_6^* C_2 + C_7^* C_3 \Big) \ , \qquad \langle I_2^y \rangle = Im\Big(\ldots \Big) \ . \tag{14c}$$

To determine the range of values of J' (second neighbor coupling constant) for which the entangled state is well defined after the two pulses, that is, where the other resonances and non-resonant transition are canceled, we calclate the fidelity paramete [10] for this process,

$$F = \langle \Psi_{expected} | \Psi_{numerical} \rangle \ , \tag{15}$$

where $\Psi_{expected}$ is our state (11), and $\Psi_{numerical}$ is the resulting wave function from our simulations. Fig. 6 shows the fidelity as a function of the ratio of the second neighbor interaction constant to first neighbor interaction constant, J'/J. As one can see, for a value $J'/J \geq 0.04$ one gets a very well defined entangled state. This means that the second neighbor interaction with even two orders of magnitud weaker than the first neighbor interaction, we can generate an entangled state in this system.

4. Conclusions and Comments

We have studied the formation of an entangled state using two pulses in a chain of three nuclear spins system with first and second neighbor Ising spin interaction. The characteritics of the entangled state were determinated, and we found that the entanglement can be realized even for very weak second neighbor spin interaction ($J'/J \geq 0.04$). We consider that the coupling constant J' may play an important rolle in the so called 2π-method found in reference [8,9] to supress non-resonant transition in the chain of nuclear spins system because this parameter will enter in the detuning parameter ($\Delta = (E_p - E_m)/\hbar - \omega$).

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Figure Captions

Fig. 1 Energy levels and resonant frequencies of interest.

Fig. 2 Entangled state formation, (1): $Re\ D_0$, (2): $Im\ D_0$, (3): $Re\ D_5$, (4): $Im\ D_5$ with $J' = 0.2$

Fig. 3 Probabilities for $J' = 0.2$, (k): $|C_k(t)|^2$ for $k = 0, \ldots, 7$.

Fig. 4 Expected values (a): $\langle I_0^z \rangle$, (b): $\langle I_1^z \rangle$, and (c): $\langle I_2^z \rangle$.

Fig. 5 For $J' = 0.2$, expected values of the transversal components of the spin.

Fig. 6 Real, Imaginary parts of the Fidelity, and its modulus.

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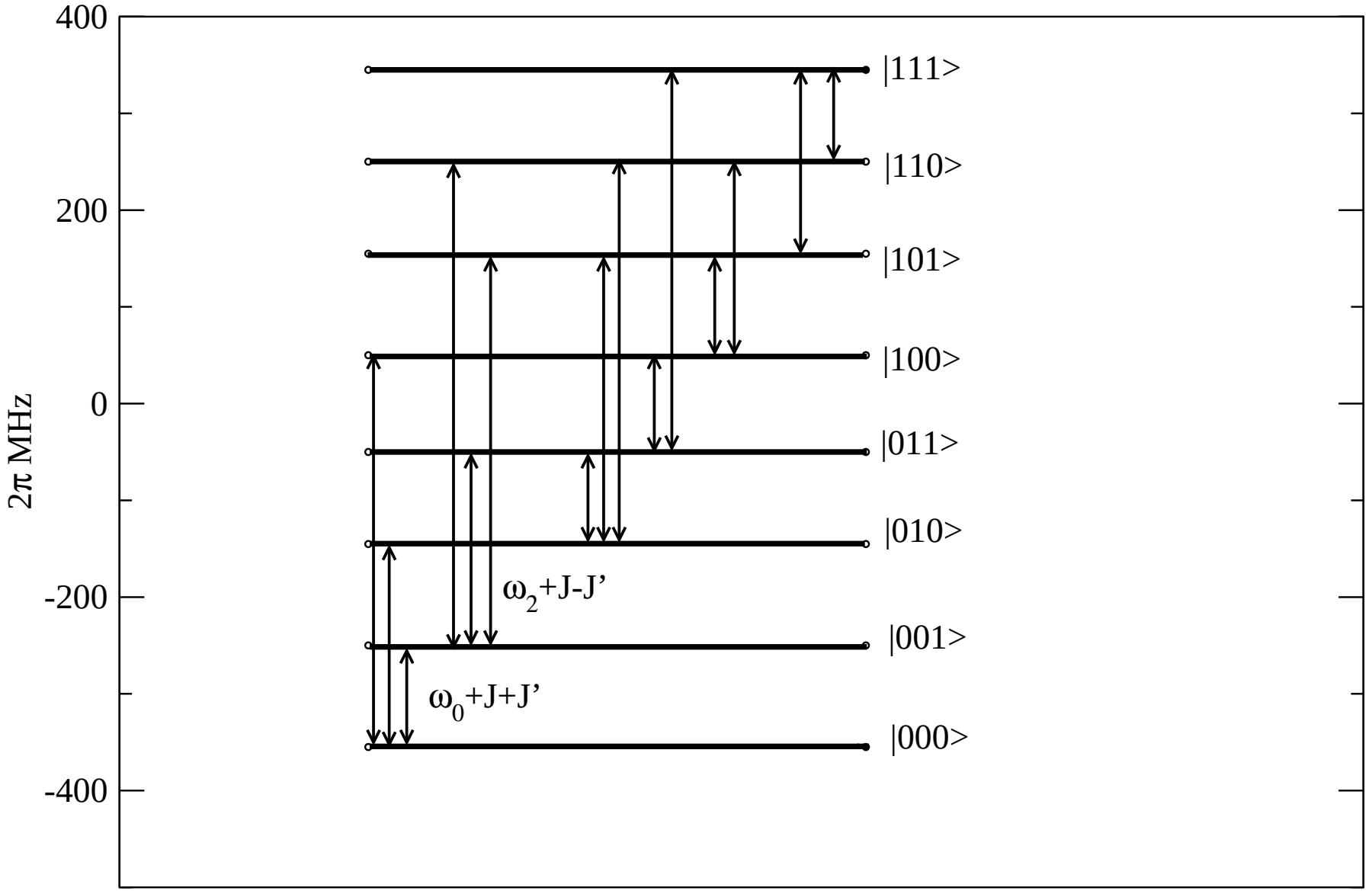
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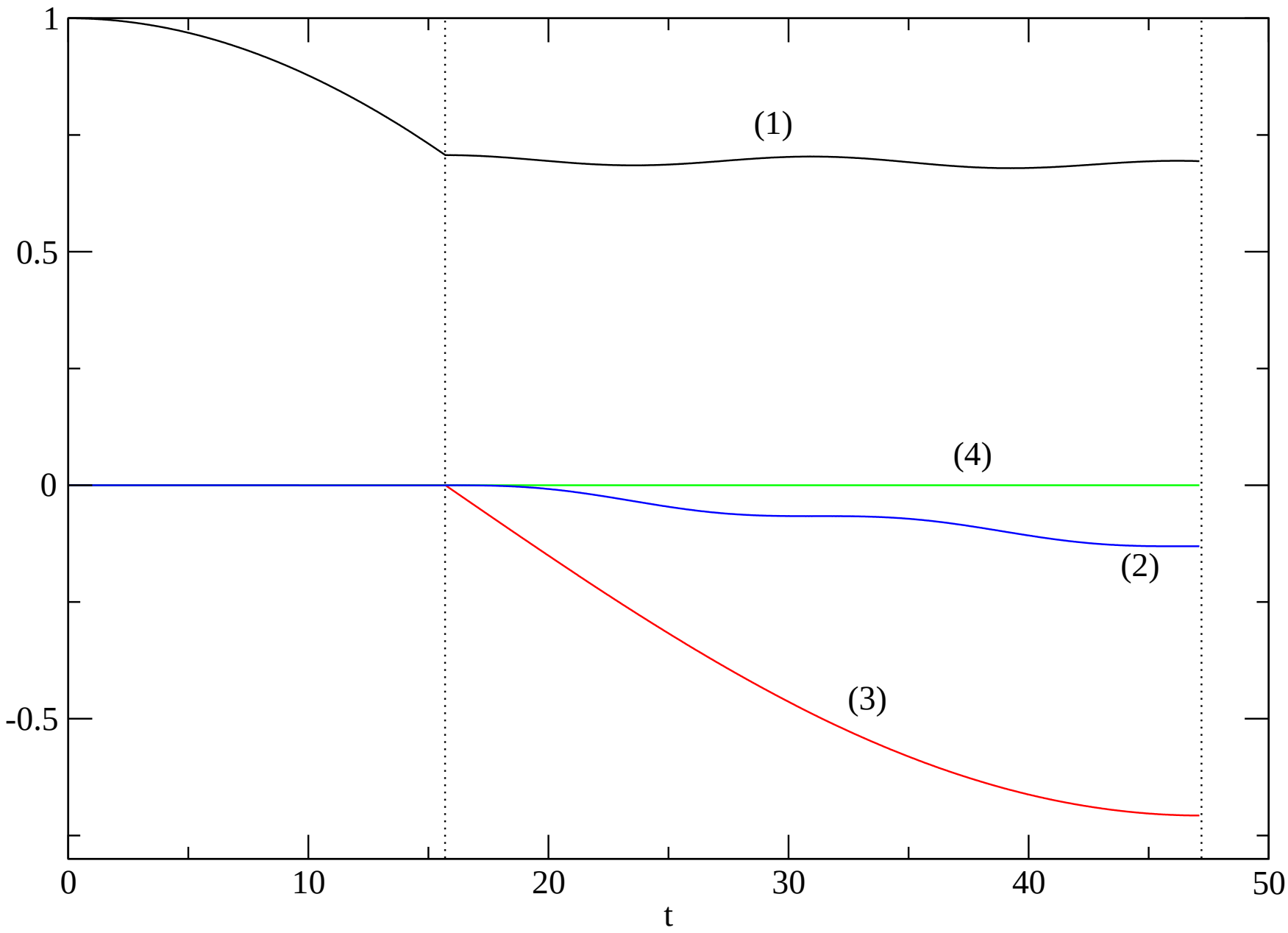
ω2+J-J'
ω0+J+J'

Fig. 1



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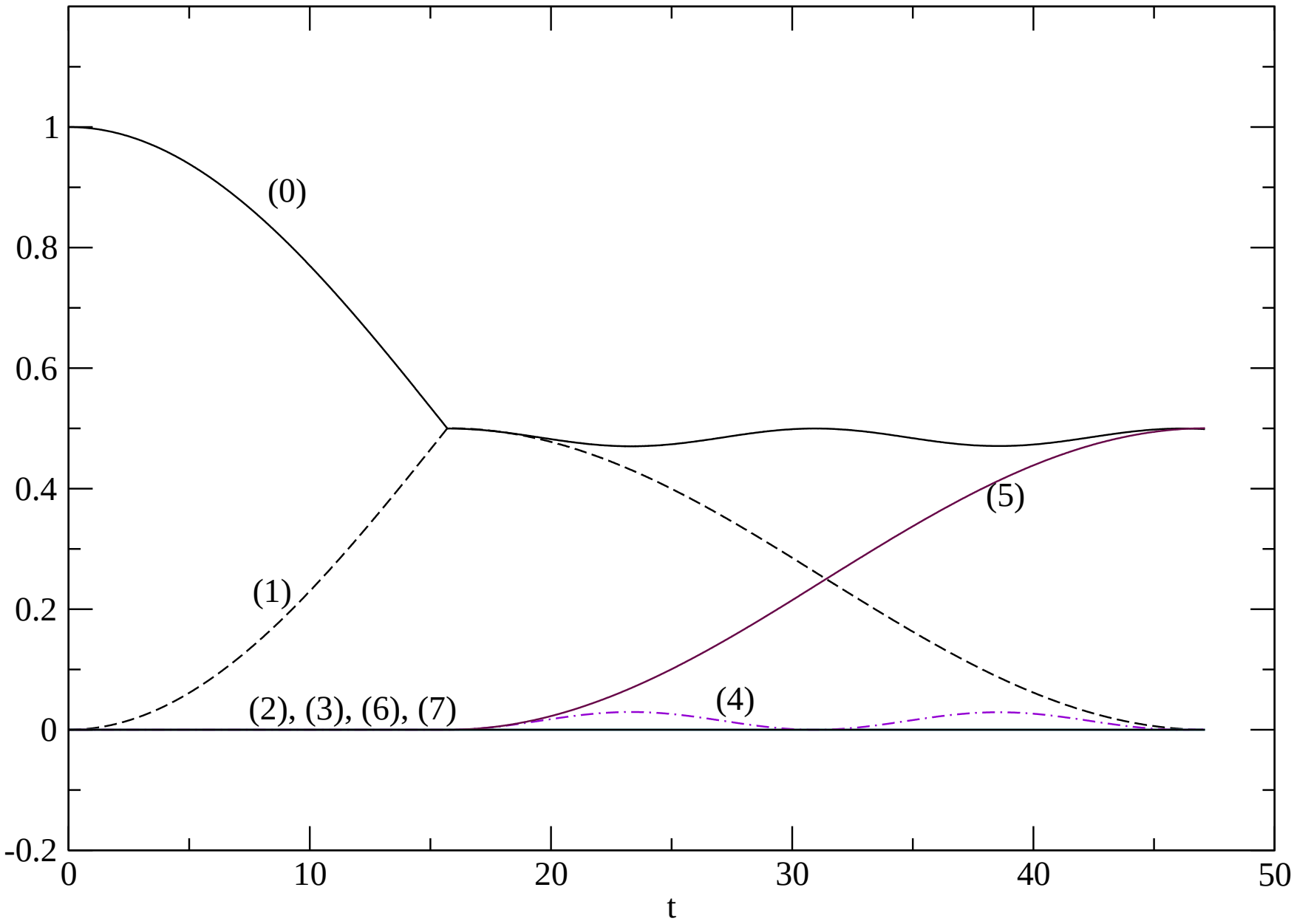

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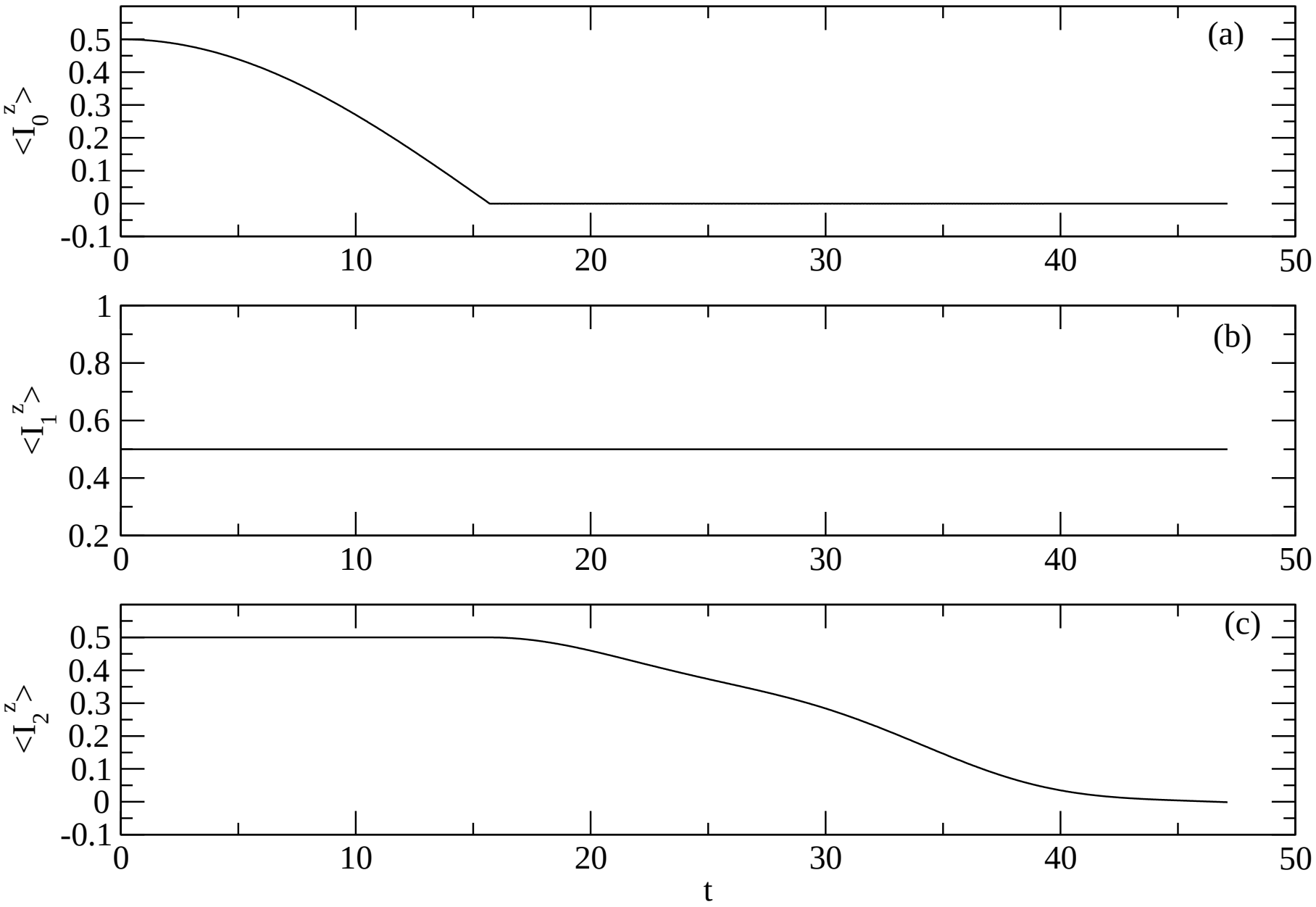
(a)
(b)
(c)
$\langle I_0^z \rangle$
$\langle I_1^z \rangle$
$\langle I_2^z \rangle$
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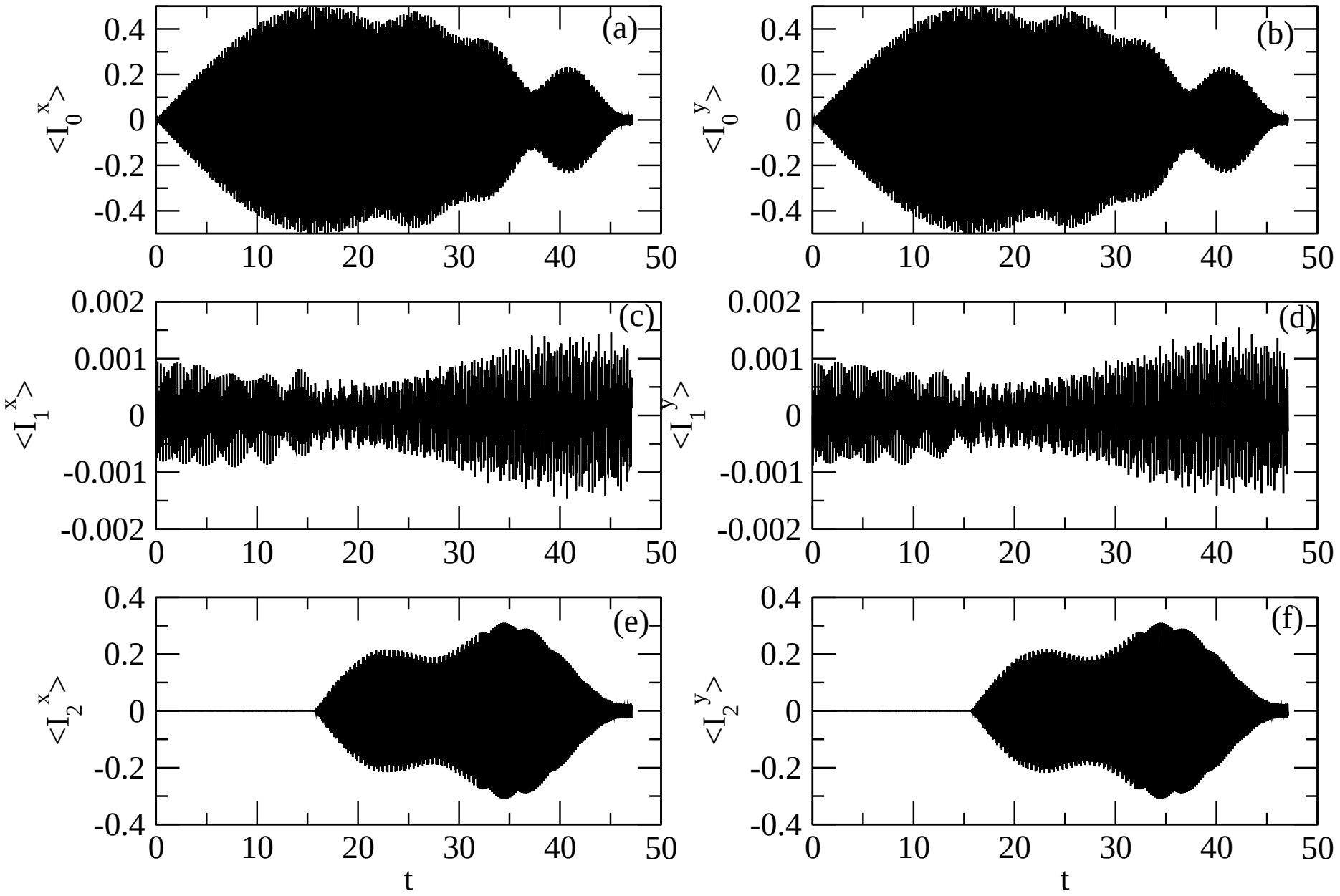
0.3
0.2
0.1
0
-0.1
1
0.8
0.6
0.4
0.2
0
10
20
30
40
50
t

Fig. 4


(a)
(b)
(c)
(d)
(e)
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-0.002
0
10
20
30
40
50
t

Fig. 5

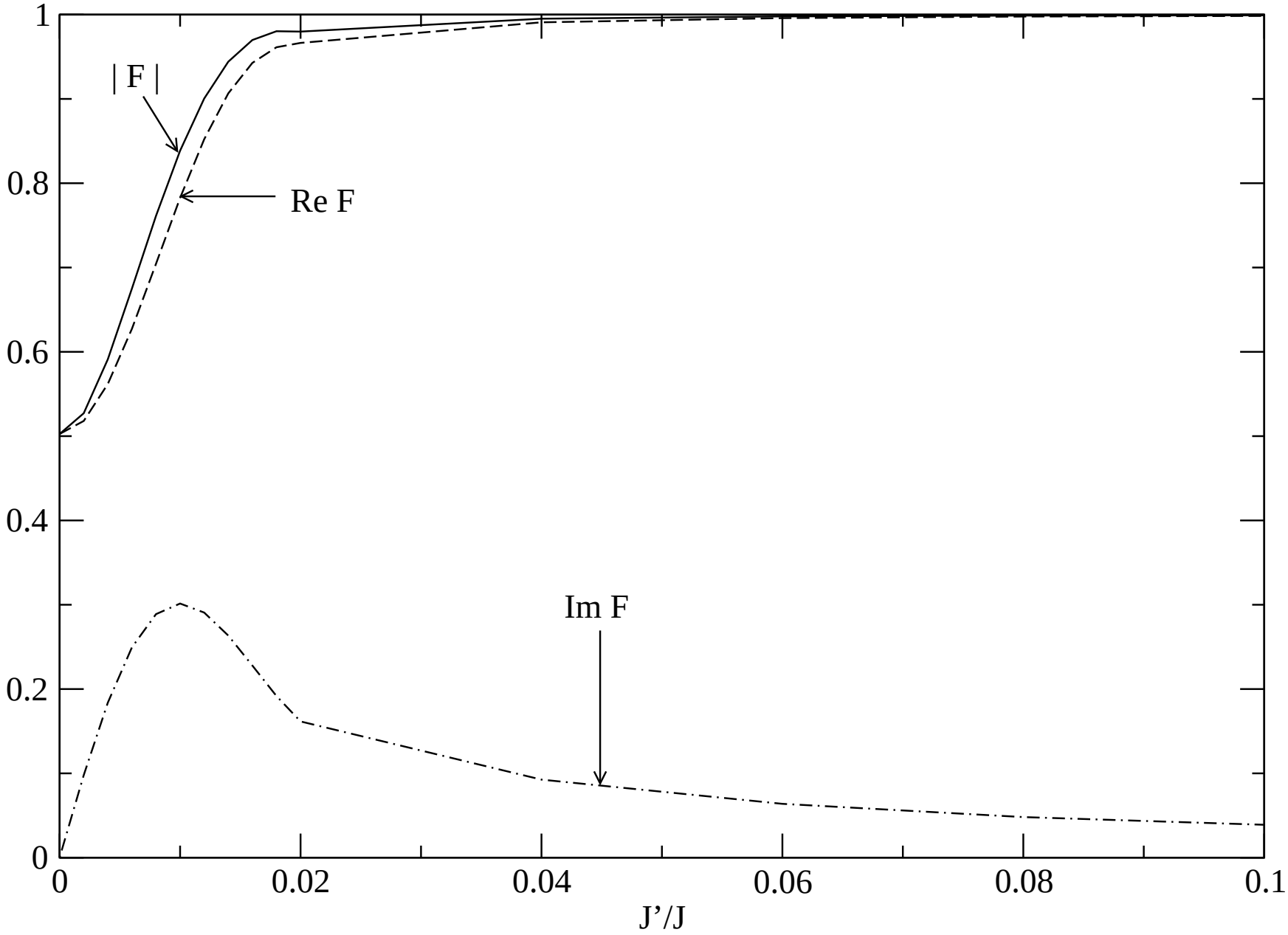

Fig. 6